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Office of Energy Efficiency & Renewable Energy

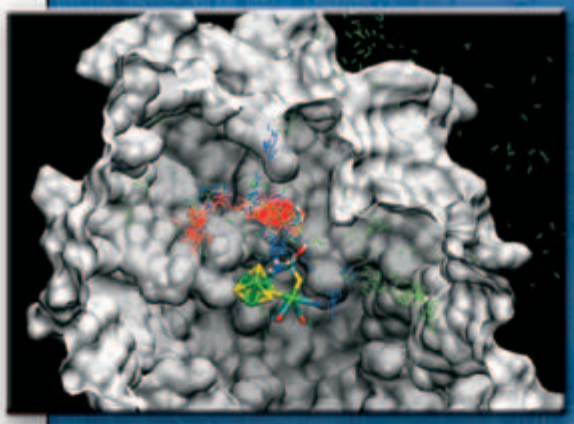
NREL National Renewable Energy Laboratory

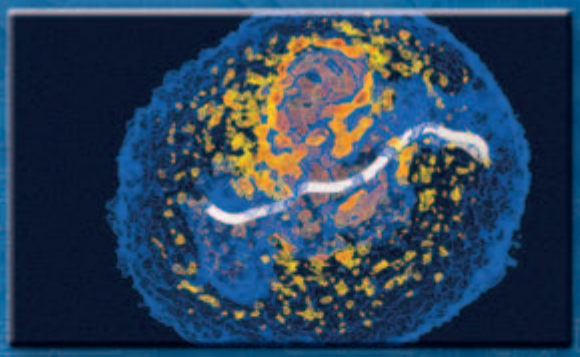
Innovation for Our Energy Future

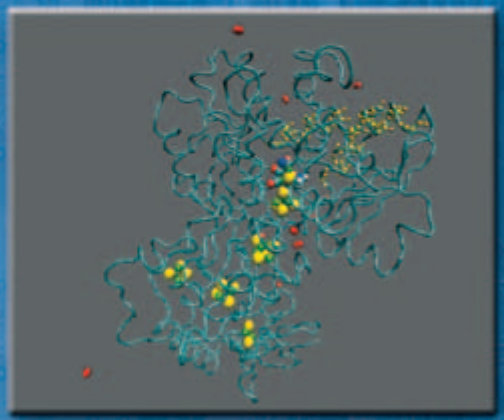
Abstracts for the Workshop on

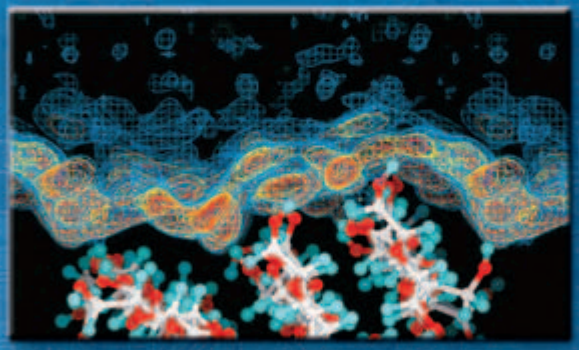
Computational Biology: Focus on Hydrogen, Biomass, and Nanoscience

Organizing Committee:
Kwiseon Kim, Wesley Jones, Mike Himmel, and Paul King









NCS 2004 • NREL Computational Sciences Workshop • September 10, 2004

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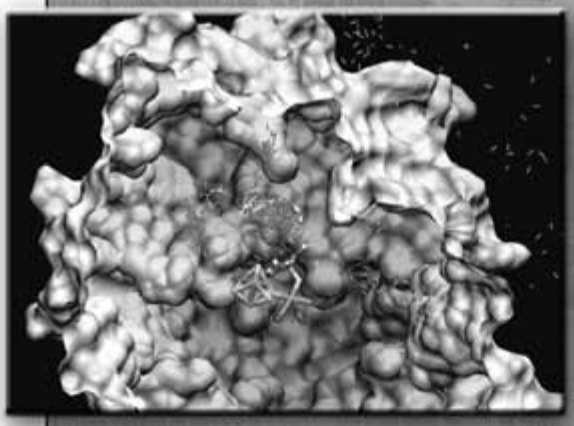

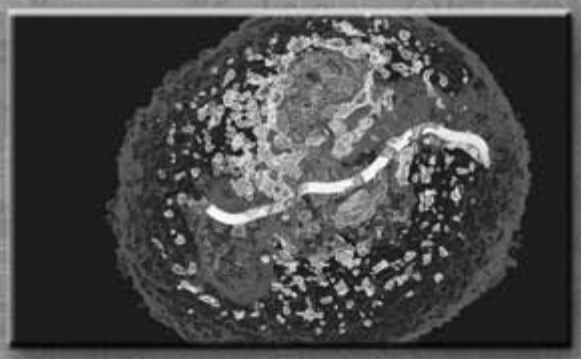

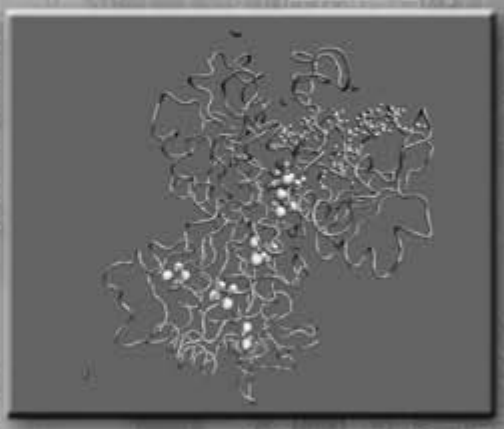

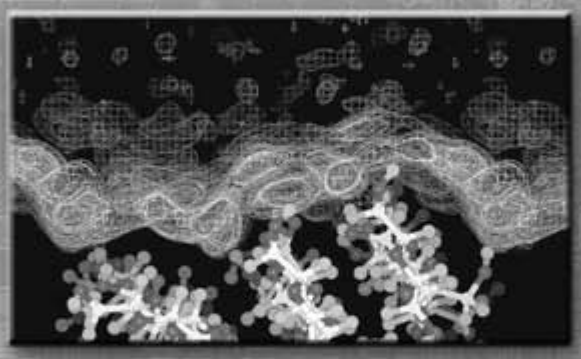

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8:00 Registration Packet and Name Tags

8:30 Stan Bull, Science & Technology Director, NREL, Opening Remarks

8:35 Session: Simulation and Modeling in Biomass Conversion

8:35 **Keynote:** John W. Brady, Cornell University and Michael E. Himmel, NREL, "Computational Modeling of Nano-Scale Cellulase/Substrate Systems"

9:20 Mark Nimlos, NREL, "Interaction of the Fungal Type I CBM with Cellulose"

9:45 Tauna Rignall, Colorado School of Mines; Clare McCabe, Vanderbilt University and Colorado School of Mines; and Michael E. Himmel, NREL, "Energetics and Conformations of the Hydrated *T. reesei* CBH I Linker Peptide"

10:10 Coffee Break

10:25 **Session: Simulation and Modeling in Photobiology**

10:25 **Keynote:** Klaus Schulten, University of Illinois, " Towards Understanding Membrane Channel"

11:10 Paul W. King, NREL; Matthew Posewitz, NREL and Colorado School of Mines; Jordi Cohen, University of Illinois; Kwiseon Kim, NREL; Maria Ghirardi, NREL; Klaus Schulten, University of Illinois; and Michael Seibert, NREL; "Hydrogen-Producing Enzymes: Exploring Structural Effects on Oxygen Tolerance"

11:35 Kwiseon Kim, NREL, "Gas Diffusion Studies Inside the CpI [Fe]-Hydrogenase"

12:00 Boxed Lunch and Discussion

1:00 **Session: Bioinformatics for Renewable Energy**

1:00 **Keynote:** Giri Chukkapalli, SDSC and Michael Crowley, The Scripps Research Institute, "Hardware and Software Concerns for Scaling New Problems in Biology"

1:45 **Keynote:** John Houghton, DOE, "Computational Challenges for Genomics: GTL Biology"

2:30 Mathew Posewitz, NREL and Colorado School of Mines, "Probing Hydrogen Production in *Chlamydomonas reinhardtii* Using Random Mutagenesis and High-Throughput Approaches"

2:55 Stan Bower, NREL, "Bioinformatics for Bioenergy: Why and How"

3:20 Coffee Break

3:35 **Session: Modeling Hard- and Soft-Matter Interfaces**

3:35 Gustavo Dalpian, Pierre Carrier, and Su-Huai Wei, NREL, "Theoretical Study of Structural, Electronic and Optical Properties of a Photovoltaic Molecular Semiconductor: Perylene Diimide"

4:00 Xianghong Qian, Colorado State University, "*Ab Initio* Molecular Dynamics Simulation of Xylose and Glucose Degradation Mechanisms in Acidic Media"

4:25 Yong-Hyun Kim, Jun Feng, Marcus Jones, Shi-You Ding, Melvin P. Tucker, Garry Rumbles, Michael E. Himmel, Michael J. Heben, and Shengbai Zhang, NREL, "Interactions Between Semiconductors and Organic Molecules such as Carbon Nanotubes, Cyclodextrins, and Amino Acids"

5:00-7:00 Reception at Solarium

Introduction

Computational science stands at the forefront of biological modeling and simulation. The challenges in this field are two-fold. First, biological computational science is obliged to use high-performance computers and advanced visualization to explore ever increasingly complex systems and datasets. Second, validation of theory with experiment is exceptionally critical in this new field.

The Computational Sciences Center (CSC) is supporting the NREL Computational Sciences Workshop (NCS 2004) on Computational Biology to facilitate understanding and enhancement of the capabilities of computational science in research as well as the needs of the more traditional methods of scientific investigation, theory and experiment. The workshop aims to bring together researchers from scientific areas studying biological systems to discuss problems and potential solutions, to identify new issues, and to shape future directions for research.

There are four technical sessions. Topics include:

- Simulation and Modeling in Biomass Conversion
- Simulation and Modeling in Photobiology
- Bioinformatics for Renewable Energy
- Modeling Hard- Soft-Matter Interfaces

Simulation and Modeling in Biomass Conversion

Computational Modeling of Nano-Scale Cellulase/Substrate Systems

John W. Brady[1] and Michael E. Himmel[2]

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[2]National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO 80401

The cellobiohydrolase (CBH) enzymes produced by fungi are considered to be the most active known glycosyl hydrolases acting on crystalline cellulose. The processive action these enzymes exhibit strongly suggests the motion of a "protein machine," and thus our objective is to gain an understanding of this mechanism at the molecular and thermodynamic level. However, a significant problem in using computer simulations to directly model the enzymatic hydrolysis of cellulose is the very large size of the systems involved. The smallest practical units of the insoluble substrate are cellulose microfibrils containing many tens of thousands of atoms, which are on the order of at least 200 nm long, and 4-6 nm in diameter. In addition, the catalytic units of cellulases are large globular proteins with many thousands of atoms. Many cellulases are found in larger complexes with substrate binding domains tethered to catalytic domains via linker peptides. The *T. reesei* CBH I cellulase, for example, contains 497 residues and has a length of over 125 Å. The large size of these components also implies that in an aqueous environment they move slowly as a result of friction with the viscous water. The large size and long timescales for these systems have been serious impediments to modeling complete systems in atomistic detail. However, with the advent of massively parallel computers, simulations which were previously infeasible become possible, at least in principle. The results of preliminary simulations of just such systems will be described. These will include a model cellulose microfibril 20 nm in length and 6 nm in diameter, containing 108 cellulose chains, each 40 glucose residues in length. This entire model was immersed in a periodic box of water containing over 100,000 molecules. An even larger system consisting of such a fibril with a complete CBH I cellulase complex bound to it in an aqueous periodic box will also be discussed. This enzyme/substrate complex contains approximately 280,000 water molecules, for a total of over 700,000 atoms. The types of information that can be obtained from such simulations will be described, and prospects for such simulations in the future will be discussed.

NOTES:

Interaction of the Fungal Type I CBM with Cellulose

Mark Nimlos
National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO 80401

The interaction of the cellulase cellulose binding modules (CBMs) with cellulose surfaces plays an important role in the processivity of the CBH I (Cel7A) enzyme. This module is known to bind the enzyme to the cellulose surface and may also assist in the decrystallization of microcrystalline cellulose. Enzymatic decrystallization of cellulose requires removal of single cellodextrins from a strong and highly organized hydrogen bonding environment. However, the binding of the CBM to the surface must also be weak enough to allow the enzyme to translate down the cellulose surface. We have initiated a molecular dynamics study of the interaction of the type I CBM with a model cellulose 1β surface using the CHARMM molecular mechanics force field. Of particular interest, revealed so far in this study, is the orientation of the aromatic residues located in the interaction space between the CBM and the cellulose surface. These residues reside on a relatively planar face of the CBM and appear to be regularly spaced. Thus, it is tempting to assume that the aromatic rings in the CBM align with the glucose rings in cellulose. We present preliminary results regarding this alignment and possible effects that may have on decrystalization. Another aspect of interest is the arrangement of water molecules around the cellulose surface before and after adsorption of the CBM. It is known that a high-density layer of water forms on neat cellulose and the disruption of this layer may be another important component of the function of the CBM.

NOTES:

Energetics and Conformations of the Hydrated *T. reesei* CBH I Linker Peptide

Tauna Rignall[1], Clare McCabe[1,2], and Michael E. Himmel[3]

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Cellobiohydrolase I (CBH1), from *Trichoderma reesei*, is one of the most active cellulases known. CBH1, only found in fungal cellulase systems, hydrolyzes cellulose in a "processive" manner, liberating cellobiose residues. It is a multi-domain enzyme, consisting of a large catalytic domain containing an active site tunnel and a small cellulose binding module joined to one another by a 27 amino acid linker peptide. Although the spatial conformation adopted by the linker peptide is yet to be determined, it is thought to play an important role in the enzymatic hydrolysis of cellulose. Since the linker peptide is relatively small, it is possible to study the energetic conformations adopted by the linker through molecular mechanics and molecular dynamics techniques. In this work, we will present results of computer simulations of the O-linked glycosylated linker peptide in an aqueous environment in order to gain insight into the role the linker may play in cellulose hydrolysis.

NOTES:

Simulation and Modeling in Photobiology

Towards Understanding Membrane Channels

Klaus Schulten

Beckman Institute and Department of Physics, University of Illinois, Champaign-Urbana IL 61801

Membrane channels are realized through proteins that form pores in the walls of living cells. The pores are optimized for high selectivity as well as high conductance, often controlled through extraneous factors (so-called gating). Selectivity and conductance can be measured with high sensitivity, even for individual channels. Recently available atomic resolution structures permit one to study channels through in-situ molecular-dynamics simulations that can determine the mechanisms underlying selectivity and conductance as well as explain in detail the relationship between channel architecture and function. The progress achieved through advances in computational technologies will be illustrated for aquaporin channels that conduct water and small alcohols and for mechanosensitive channels that protect cells against osmotic shock. The conceptual and practical convergence of channel biology and device physics will be illustrated through measurements and simulations of synthetic nanopores that hold promises for cost-effective DNA sequencing.

NOTES:

Hydrogen-Producing Enzymes: Exploring Structural Effects on Oxygen Tolerance

Paul W. King[1], Matthew Posewitz[1,2], Jordi Cohen[3], Kwiseon Kim[1],
Maria Ghirardi[1], Klaus Schulten[3], and Michael Seibert[1]

[1]National Renewable Energy Laboratory, Golden CO, 80401
[2]Colorado School of Mines, Golden, CO, 80401
[3]Beckman Institute, University of Illinois, Champaign-Urbana IL 61801

Photobiological H_2 production by the green alga *Chlamydomonas reinhardtii* is being investigated at NREL for its potential use as a renewable H_2 production system. Under normal growth conditions, H_2 metabolism by *C. reinhardtii* is a strictly anaerobic process that occurs as cells transition from dark/anaerobic conditions to light/aerobic conditions. A principle cause of the transient nature of H_2 metabolism during the initial stages of photosynthesis is the rapid inactivation of the [Fe]-hydrogenase by O_2. Thus, development of an efficient, large-scale, photobiological H_2-production system requires addressing the O_2 sensitivity of algal [Fe]-hydrogenases. To better characterize the process of O_2 inactivation we are investigating the structural and functional properties of algal [Fe]-hydrogenases and homologous bacterial [Fe]-hydrogenases to identify elements critical to O_2 sensitivity. These experimental studies are being complemented by a systematic computational approach aimed at identifying O_2-diffusion pathways. Results of these investigations are guiding the iterative modification of [Fe]-hydrogenases with the aim of designing enzymes with improved O_2 tolerance.

NOTES:

Gas Diffusion Studies Inside the CpI [Fe]-Hydrogenase

Jordi Cohen[1], Kwiseon Kim[2], Paul W. King[2], Klaus Schulten[1], Maria L. Ghirardi[2], and Michael Seibert[2]

[1]Beckman Institute, University of Illinois, Urbana-Champaign, Illinois 61801, U.S.A.
[2]National Renewable Energy Laboratory, Golden, Colorado 80401, U.S.A

The photobiological conversion of H_2O into H_2 by the green algae C*hlamydomonas reinhardtii* offers a promising system for the production of clean, renewable H_2. However, the rapid deactivation of the catalytic site, which is buried inside the algal [Fe]-hydrogenase, by atmospheric O_2 poses a serious obstacle to an economical, large-scale H_2 production system. All-atom computer simulations of the diffusion process of small gaseous inhibitors inside a hydrogenase protein can provide answers as to how to engineer the hydrogenase to be more resistant to O_2 deactivation. We have carried out simulations of the diffusion of the O_2 inhibitor and the H_2 product inside a model of the homologous CpI [Fe]-hydrogenase from *Clostridium pasteurianum* obtained from X-ray crystallography. Preliminary results suggest that O_2 can enter and exit the enzyme through a finite number of paths consisting of connected cavities. These areas of high O_2 occupancy during our simulations correlate well with pre-existing "packing defects" present in the crystal structure. The much smaller H_2, on the other hand, can more freely diffuse throughout the protein. These results suggest that, in theory, it is possible to increase the O_2 tolerance of [Fe]-hydrogenases by limiting O_2 diffusion without preventing the H_2 product from being released by the protein. By targeting mutations to the O_2 pathway-lining residues, O_2 diffusion within the protein could be reduced while H_2 outward diffusion would be unaffected. Eventually, we wish to extend the knowledge gained from modeling and simulation of the bacterial CpI [Fe]-hydrogenase towards engineering of the highly homologous [Fe]-hydrogenase from *Chlamydomonas reinhardtii.*

NOTES:

Bioinformatics for Renewable Energy

Hardware and Software Concerns for Scaling New Problems in Biology

Giri Chukkapalli[1] and Micheal Crowley[2]

[1]San Diego Supercomputer Center, University of California San Diego, La Jolla, CA 92093
[2]The Scripps Research Institute, La Jolla, CA 92037

We are excited about the advent of new architectures that provide massive amounts of computing power. The questions from biophysics, structural biology, biochemistry that have been only dreams in the computational chemist's mind are on the verge of being realistically studied. For some problems, the computing power and tools are already available, while for others, there is enough raw computing power but the tools are either ill-suited to the current architectures or do not exist yet. Still others are simply still not realizable with the currently available hardware.

Our presentation gives an overview of what is currently possible and what is becoming possible with new hardware and software including examples of problems and systems that we are studying and are aiming at studying. Structure and function, of large multi-macromolecular systems are a primary focus: enzyme-substrate complexes, membrane systems like ion channels, virus capsids, and ribosomes to name a few. We present the obstacles to harnessing the latest computing power from various architectures for molecular mechanics and dynamics studies and what we see as realistic goals for the immediate and near future.

This talk consists of two parts. First, we present the computational characteristics of the biology applications along with the current state-of-the-art High-End-Computing (HEC) hardware and software resources available to the computational biologist. We will also give a brief overview of what will be coming in the future, such as IBM BlueGene and DARPA PERCS mahchines.

In the second part, we address more specific efforts underway at SDSC and SCRIPPS in retargetting general purpose MD tools, CHARMM and AMBER, for solving large-scale systems on the above mentioned HEC platforms. By using the NREL's 1 million atom cellulase simulation problem as an example, we present some performance analysis and some preliminary scaling numbers.

NOTES:

Computational Challenges for Genomics: GTL Biology

John Houghton, U.S. Department of Energy, Washington, DC 20585

NOTES:

Probing Hydrogen Production in *Chlamydomonas reinhardtii* Using Random Mutagenesis and High-Throughput Approaches

Matthew C. Posewitz[1, 2], Paul W. King[1], Sharon L. Smolinski[1], Liping Zhang[1], Maria L. Ghirardi[1], Michael Seibert[1]

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The eukaryotic green alga, *Chlamydomonas reinhardtii*, produces H_2 under anaerobic conditions, in a reaction catalyzed by reversible hydrogenases. In order to identify genes that influence H_2 production in *C. reinhardtii*, a library of 6,000 colonies on agar plates (provided by Prof. A. Melis, University of California, Berkeley), was screened with sensitive chemochromic H_2-sensor films for clones defective in H_2 production. Two mutants of particular interest were fully characterized. One mutant, *hydEF-1*, is unable to assemble an active [Fe]-hydrogenase. This is the first reported *C. reinhardtii* mutant that is incapable of producing any H_2. The second mutant, *sta7-10*, is unable to accumulate insoluble starch and has drastically reduced H_2-photoproduction rates in comparison to the wild-type. In *hydEF-1*, anaerobiosis induces transcription of the two reported *C. reinhardtii* hydrogenase genes, *HydA1* and *HydA2*, indicating a normal transcriptional response to anaerobiosis. In contrast, the induction of both hydrogenase genes in *sta7-10* is significantly attenuated. Global gene expression in these two mutants will be compared to the wild-type using cDNA microarrays. This information will lead to a better understanding of the biochemical networks that support H_2 production in *C. reinhardtii*. Sophisticated computational approaches will be necessary to interpret the vast amount of data generated by the microarray experiments. This information will subsequently be leveraged in molecular engineering experiments aimed at enhancing H_2 production in *C. reinhardtii*. This work was supported by the Division of Energy Biosciences, Office of Science, U.S. Department of Energy, and by the Hydrogen, Fuel Cells, and Infrastructure Technologies Program, U.S. Department of Energy.

NOTES:

Bioinformatics for Bioenergy: Why and How

Stan Bower
National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO 80401

NOTES:

Modeling Hard- and Soft-Matter Interfaces

Theoretical Study of Structural, Electronic and Optical Properties of a Photovoltaic Molecular Semiconductor: Perylene Diimide

Gustavo M. Dalpian, Pierre Carrier, and Su-Huai Wei
Basic Sciences, National Renewable Energy Laboratory, Golden, CO 80401

Organic semiconductors that build upon organic molecular building blocks are being increasingly employed for the fabrication of electronic materials due to their processability, flexibility, and structural diversity. They are promising materials for making low-cost and large-scale optoelectronic devices such as light-emitting diodes, flexible displays, and solar cells. Although many studies have been carried out in understanding the physical properties of these fascinating semiconductors, first-principles band-structure calculations of these systems are still quite rare due to the complexity of these materials, and many fundamental material properties of these semiconductors are still not well known. For example, PPEEB, a perylene diimide derivative, which crystallizes in a highly ordered and periodic solid at room temperature, is a promising candidate for organic photovoltaic solar cells. However, further improvement of the solar cell efficiency using this material requires a better understanding of its doping and transport properties and their relation with the crystal structure. In this work, using the state-of-the-art density functional theory within the local density approximation (LDA) we have studied the structural, electronic and optical properties of PPEEB. Based on some experimental parameters and minimizing the quantum mechanical forces, we propose a structural model for the arrangement of solid PPEEB. Our calculations show that the valence band maximum (VBM), or HOMO, and the conduction band minimum (CBM), or LUMO, states are localized in two different regions of the solid: the VBM wavefunction is localized in the radical tails, while the CBM is in the perylene core. The calculated fundamental band gap is ~0.5 eV. However, due to the small overlap of the VBM and the CBM states, the calculated optical band gap is at ~1.1 eV, which corresponds to a transition between the CBM and a low-lying valence band state with wave-function localized also in the perylene core region. We propose that this optical band gap should be compared with the experimentally measured optical excitation at ~2 eV. The smaller calculated value at ~1.1 eV is a typical LDA band-gap error for semiconductors. We suggest that the presence of the tail states above the HOMO states of the perylene core will have large effects-on the doping and transport properties of this semiconductor. For instance, it reduces the carrier recombination rate, but also makes the p-type doping in the core region much more difficult.

NOTES:

Ab Initio Molecular Dynamics Simulation of Xylose and Glucose Degradation Mechanisms in Acidic Media

Xianghong Qian
Colorado State University, Fort Collins, CO 80523

Sugar degradation during pretreatment of biomass in an acidic media reduces xylose and glucose yields and is a serious economical concern. It is known that furfural and hydroxymethylfurfural (HMF) are the degradation products from xylose and glucose, respectively. However, these two products can only partially account for the sugar loss commonly observed. Moreover, detailed mechanisms for the most critical sugar degradation reactions are still controversial. Researchers have recently speculated about the existence of parasitic reaction pathways to form other byproducts. We have employed ab initio molecular dynamics simulation to elucidate xylose and glucose degradation pathways. In the case of xylose, a 2,5-anhydride intermediate was observed leading to the formation of furfural through further elimination of water. This pathway agrees with the mechanism proposed by Antal and coworkers in that no open chain intermediates were found. In the case of glucose, a series of intermediates were observed before forming 2,5-anhydride that eventually leads to HMF. One of these intermediates was a very short-lived (< 100 femtoseconds) open-chain form. Furthermore, two additional side-reaction pathways were identified which lead to degradation products other than HMF. These side-reactions may be explained by the probability that protons could potentially attack all five of the glucose ring OH groups, yet only one of those events lead to the formation of HMF. In this regard, the differences between xylose and glucose acid-degradation mechanisms will be discussed.

NOTES:

Interactions Between Semiconductors and Organic Molecules such as Carbon Nanotubes, Cyclodextrins, and Amino Acids

Yong-Hyun Kim[1], Jun Feng[2], Marcus Jones[1], Shi-You Ding[2], Melvin P. Tucker[2], Garry Rumbles[1], Michael E. Himmel[2], Michael J. Heben[1], and Shengbai Zhang[1]

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Colloidal semiconductor quantum dots can be assembled through organic molecular linkers such as carbon nanotubes and proteins for application to high-efficiency photo-energy conversion. In order to understand the physics and chemistry of the interfaces between the colloidal semiconductors and the organic linkers, we have performed first-principles density functional theory calculations about the simplified interfaces of flat semiconductor surfaces and units of long-chain organic molecules, e.g., carbon nanotubes, glucoses, and amino acids. For carbon nanotubes as ideal linkers because of various electronic properties from genuine metals to moderate band gap semiconductors, we have identified band offsets, adsorption energy, charge transfer, and surface-induced bipolar doping of zigzag carbon nanotubes on InAs, GaAs (III-V), CdSe (II-VI) and Si (IV) surfaces. We found the approximately universal alignment of the graphene Fermi level (i.e., mid-gap) of nanotubes throughout the semiconductor band gaps. In case of polarized semiconductor surfaces, there exists a strong dipole field effect that may cause significant charge transfer from/to nanotubes. We also study theoretically adsorption characteristics of cyclodextrins, glucoses, sodium hydroxyls, and amino acids with CdSe/ZnS core-shell colloidal quantum dots, which can be brought into water by those organic molecular ligands. We have found that hydroxyls from glucoses and simple bases can react with the ZnS surface effectively by exchanging the oxygen atom with surface sulfur atoms. This mechanism naturally explains the strong binding of those molecules and thus the ~17-nm red shift of the photoluminescence peak of the modified core-shell quantum dots in experiments. We have also found that some amino acids are as good in passivating the quantum dots as the conventional TOP and TOPO molecules.

NOTES:

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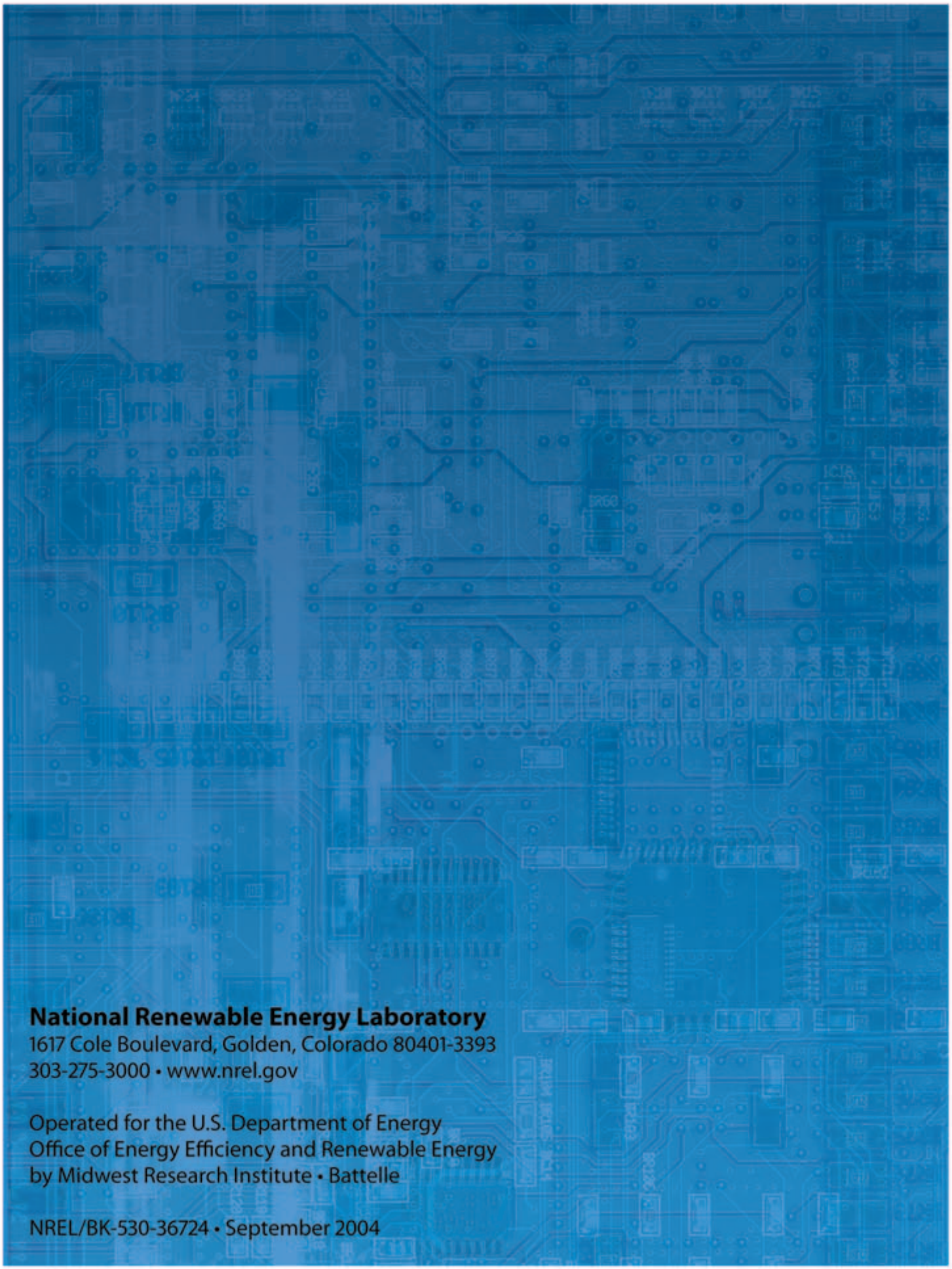

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